

Dynamical Mean-Field Theory — from Quantum Impurity Physics to Lattice Problems

Ralf Bulla

*Theoretische Physik III, Elektronische Korrelationen und Magnetismus,
Universität Augsburg, 86135 Augsburg, Germany*

Abstract

Since the first investigation of the Hubbard model in the limit of infinite dimensions by Metzner and Vollhardt, dynamical mean-field theory (DMFT) has become a very powerful tool for the investigation of lattice models of correlated electrons. In DMFT the lattice model is mapped on an effective quantum impurity model in a bath which has to be determined self-consistently. This approach lead to a significant progress in our understanding of typical correlation problems such as the Mott transition; furthermore, the combination of DMFT with ab-initio methods now allows for a realistic treatment of correlated materials. The focus of these lecture notes is on the relation between quantum impurity physics and the physics of lattice models within DMFT. Issues such as the observability of impurity quantum phase transitions in the corresponding lattice models are discussed in detail.

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INTRODUCTION

Strongly correlated electron systems have been one of the most important topics in theoretical solid state research over the past decades. The major challenge in these systems is that interesting features (like the Mott transition, Gebhard (1997), Imada (1998)) typically occur at intermediate coupling strengths, so that perturbative approaches cannot be applied. Although a number of *non*-perturbative techniques have been developed for correlated electron systems, we are still far away from a complete understanding of models like the two-dimensional Hubbard model, let alone an exact solution of these models.

In the past 15 years, considerable progress has been achieved through the development and application of the dynamical mean-field theory (DMFT) (Georges *et al.* 1996, Metzner and Vollhardt 1989). One of the reasons for this success is that in the standard implementation of DMFT, a lattice model is mapped on a quantum impurity model, for which very powerful, non-perturbative methods are already available (Hewson 1993). This quantum impurity model consists of a single correlated site in a free fermionic bath whose structure has to be determined self-consistently.

DMFT is exact in the limit of infinite coordination number (or infinite dimensions). For any finite-dimensional system, DMFT is an approximation as it fails to take into account non-local fluctuations. Nevertheless, it can be used as a reasonable starting point in many cases. In particular, a variety of cluster extensions of DMFT are currently developed (for a review see Maier *et al.* (2004)).

Extensive reviews on various aspects of DMFT have already been published. The review by Georges *et al.* (1996) gives a detailed account of the technical issues and early applications such as the investigation of the Mott transition (see also the lecture notes by Georges (2004) and more recent work on the Mott transition (Bulla *et al.* 2001, Georges *et al.* 2004)). A brief overview of DMFT is given in the Physics Today article by Kotliar and Vollhardt (2004), which also gives an introduction to the combination of ab-initio methods with DMFT (for a review see Held *et al.* (2003)).

Here, we do not attempt to give an overview of all the technical issues and the various applications of DMFT. Instead, the focus of this paper is on the relation between the lattice models and the quantum impurity models on which the lattice model is mapped within DMFT. Very often, this relation is seen from the following viewpoint: let us start with a

given lattice problem, and within DMFT all that is left to do is to choose an appropriate “impurity solver” which can then be used as a black box within the DMFT self-consistency to arrive at the physics of the lattice model. [It will be evident from reading the remainder of the paper that the author regards the expression “impurity solver” as inadequate, if not misleading, as it does neither give justice to the technique one is referring to, which very often has its own intellectual merits, nor to the effective impurity model which deserves more attention instead of just being “solved”.] An alternative viewpoint is to start from quantum impurity models in general, keeping in mind the enormous variety of physical behaviour one can observe in these models, and then ask the question whether this richness can also be observed in the lattice counterparts within DMFT.

This is the viewpoint taken in this paper, discussed in detail in the section entitled “DMFT and Quantum Impurity Physics”; there we introduce and classify a variety of different quantum impurity models, with the impurity coupling to fermionic and/or bosonic baths. Of particular importance are impurity quantum phase transitions and their possible counterparts in lattice models. Before that, we give a short introduction to DMFT where we also discuss the emergence of a quantum impurity model (the single-impurity Anderson model) in the DMFT for the Hubbard model. Finally, we summarize the main conclusions of the paper and discuss the present status and future prospects of DMFT.

DMFT ESSENTIALS

Metzner and Vollhardt (1989) have shown that a non-trivial limit of infinite spatial dimensions can be defined for lattice fermion models, provided that the model parameters are appropriately scaled with the dimension. For the Hubbard model (Gutzwiller 1963, Hubbard 1963, Kanamori 1963)

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (1)$$

this scaling only involves the hopping matrix element $t = t^*/\sqrt{d}$, with t^* fixed, while the local Coulomb repulsion U is unchanged. An important consequence of this scaling is that the self-energy $\Sigma_{ij}(\omega)$ becomes purely local. This can be understood from a simple counting argument for the self-energy diagrams as shown, for example, in Fig. 1.

In this figure, the dashed lines denote the Coulomb repulsion U and the solid lines the

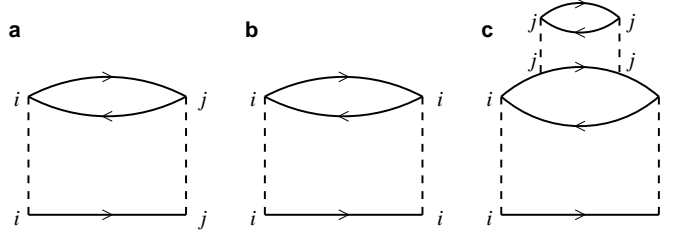


FIG. 1: Self-energy diagrams for the Hubbard model.

bare propagator $G(\omega)$. For i and j nearest neighbours in Fig. 1a, the three propagators each contribute a factor of t to the diagram, i.e., a factor of $d^{-3/2}$. With the number of nearest neighbours proportional to d , the sum of these self-energy diagrams vanishes as $d^{-1/2}$ in the limit of $d \rightarrow \infty$.

Only local diagrams as in Fig. 1b and c survive in the limit $d \rightarrow \infty$. This does not mean that the Hubbard model is reduced to a purely local model, as the propagation through the lattice is still possible (dressed only with local self-energy terms, as shown, for example, in Fig. 1c).

The local self-energy of the Hubbard model obtained in this way resembles that of a single-impurity Anderson model, which is local anyway, as the Coulomb interaction U in the Anderson model only acts on a single site. The Hamiltonian of the single-impurity Anderson model reads:

$$H = \sum_{\sigma} \varepsilon_f f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{k\sigma} V \left(f_{\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} f_{\sigma} \right). \quad (2)$$

With a proper definition of the bare propagator \tilde{G} as

$$\tilde{G}^{-1} = G_{\text{loc}}^{-1} + \Sigma_{\text{HM}}, \quad (3)$$

(G_{loc} is the local Green function of the Hubbard model) the self-energy functional $\Sigma_{\text{AM}}[\tilde{G}]$ of the Anderson model gives exactly the self-energy of the Hubbard model. The bare propagator \tilde{G} itself depends on Σ_{HM} so that we arrive at a self-consistent procedure for the calculation of the self-energy of the Hubbard model (for details, see Georges *et al.* (1996)).

Note that, although the above argument seems to be based on a perturbative expansion of the self-energy, the connection between the self-energies of the impurity and the lattice

model is *non*-perturbative. This has been shown, for example, in Potthoff (2004) where a non-perturbative construction of the Luttinger-Ward functional has been used (another non-perturbative construction is the cavity method discussed in Georges *et al.* (1996)). This means that the mapping is valid in the whole parameter space of the lattice model, even if the perturbative expansion of the self-energy has a finite radius of convergence.

The non-trivial part of this self-consistent procedure is the calculation of the self-energy of an effective single-impurity Anderson model, for which the Green function for $U = 0$ is equal to \tilde{G} . This can be achieved using a variety of techniques and the book of Hewson (1993) gives a fairly complete overview of these methods in the context of the Kondo problem. Note that the full frequency dependence of the self-energy $\Sigma_{\text{AM}}(\omega)$ needs to be calculated for the effective impurity model. Consequently, the Bethe ansatz (Hewson 1993) cannot be applied in the context of the DMFT because its ability to calculate exact results for quantum impurity problems is restricted to static quantities.

The following (incomplete) list includes those methods which have already been applied within DMFT:

- quantum Monte Carlo (Georges *et al.* 1996, Jarrell 1992);
- iterated perturbation theory (Georges and Kotliar 1992, Georges *et al.* 1996);
- non-crossing approximation (Maier *et al.* 2004, Pruschke *et al.* 1993);
- exact diagonalization (Caffarel and Krauth 1994, Georges *et al.* 1996);
- numerical renormalization group (Bulla *et al.* 1998, 2001);
- local moment approach (Smith *et al.* 2003, Vidhyadhiraja and Logan 2004);
- density matrix renormalization group (Garcia *et al.* 2004, Nishimoto *et al.* 2004);
- projective quantum Monte Carlo (Feldbacher *et al.* 2004);

(for further information, please follow the references in brackets). Interestingly, the development of DMFT lead to a renewed search for methods to calculate dynamic quantities of quantum impurity systems. New developments are the local moment approach, the (dynamic) density matrix renormalization group, and the projector quantum Monte Carlo

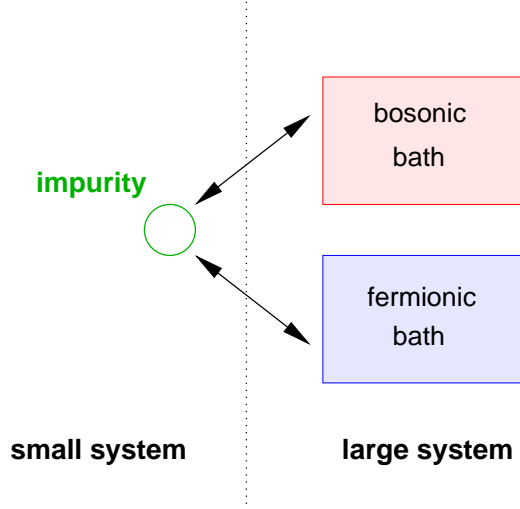


FIG. 2: In a quantum impurity system a small system (the impurity) is coupled to a large system of fermions and/or bosons (the bath).

method. For a recent overview of techniques, in particular in the context of multi-band models, see Sec. III in Maier *et al.* (2004).

To conclude this section, we want to stress again the remarkable fact that DMFT allows a mapping from a lattice model onto a quantum impurity model; from this it follows immediately that a thorough understanding of these quantum impurity models is a prerequisite for a successful investigation of lattice models within DMFT.

DMFT AND QUANTUM IMPURITY PHYSICS

Consider a quantum system with a finite number of internal degrees of freedom (the impurity) coupled to an infinite system of non-interacting fermions or bosons with a continuous density of states (the bath). An abstract view of such a *quantum impurity system* is given in Fig. 2. The impurity part of the Hamiltonian might have a complicated structure (with, for example, two-particle terms due to the Coulomb repulsion between two fermions at the impurity site as in eq. (2)) but we usually require the number of degrees of freedom of the impurity to be small enough for a solution by exact diagonalization. Due to the coupling between impurity and bath, the technical difficulty in solving such a quantum impurity problem is given by both the structure of the impurity term and the continuous spectrum of the bath.

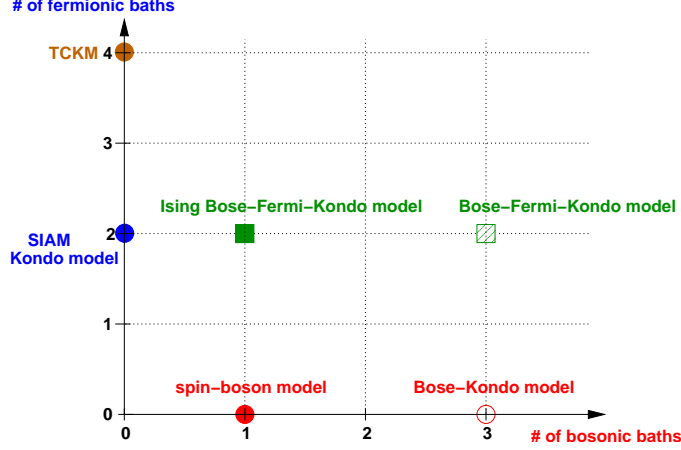


FIG. 3: Two-dimensional diagram for a classification of quantum impurity systems by counting the number of fermionic and bosonic baths to which the impurity couples.

A possible way to classify quantum impurity systems is to count the number of baths to which the impurity couples. The bath can be either fermionic or bosonic, so we arrive at a two-dimensional diagram as in Fig. 3.

The single-impurity Anderson model (SIAM) of eq. (2) occupies the point (0, 2) in this diagram as the impurity couples to *two* fermionic baths (spin \uparrow and spin \downarrow), but no bosonic bath. As discussed above, the single-impurity Anderson model appears as an effective model in the DMFT self-consistency of the single-band Hubbard model. Multi-band generalizations of the Hubbard model with, for example, an additional orbital index $\alpha = 1, \dots, M$ map onto effective impurity models occupying the points (0, $2M$) in Fig. 3.

One possible representative of the point (1, 0) in Fig. 3 is the spin-boson model with the Hamiltonian:

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_i \omega_i a_i^\dagger a_i + \frac{\sigma_z}{2} \sum_i \lambda_i (a_i + a_i^\dagger). \quad (4)$$

This model naturally arises in the description of quantum dissipative systems (Leggett *et al.* 1987, Weiss 1999). The dynamics of the two-state system, represented by the Pauli matrices $\sigma_{x,z}$, is governed by the competition between the tunneling term Δ and the friction term $\lambda_i(a_i + a_i^\dagger)$; the term $\frac{\epsilon}{2}\sigma_z$ represents an additional bias. The operators $a_i^{(\dagger)}$ constitute a bath of harmonic oscillators responsible for the damping, characterized by the bath spectral function

$$J(\omega) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i). \quad (5)$$

The so-called Bose-Kondo model (Sengupta 2000, Smith and Si 1999) at $(3, 0)$ can be viewed as a $SU(2)$ -symmetric generalization of the spin-boson model.

In the models at the points $(1, 2)$ and $(3, 2)$, the impurity couples to both fermionic and bosonic baths. These so-called Bose-Fermi Kondo models appear in various physical systems and their connection to DMFT is discussed further below.

It is important to note that each point in the diagram of Fig. 3 contains a variety of different models (with possibly different physical behaviour) as the diagram does not distinguish between different structures of the impurity and different densities of states of the bath. For example, the point $(0, 4)$ is occupied by the two-channel Kondo model (TCKM) with its well-known non-Fermi liquid fixed point (Cox and Zawadowski 1998), *and* the $SU(4)$ single-impurity Anderson model which has a Fermi liquid ground state (Hewson 1993).

In any case, the classification of Fig. 3 turns out to be useful for those (numerical) methods in which the computational effort depends mainly on the number of baths (fermionic or bosonic). This holds for those methods which are based on an actual diagonalization of bath degrees of freedom (exact diagonalization, numerical renormalization group, and density matrix renormalization group). As an example, the calculation of dynamic quantities within the numerical renormalization group (Wilson 1975) is currently restricted to the points $(1, 0)$ (Bulla *et al.* 2003, 2004), $(0, 2)$ (Bulla *et al.* 1998, Costi *et al.* 1994, Frota and Oliveira 1986, Hewson 1993, Sakai *et al.* 1989), and $(0, 4)$ (Anders 2004, Pruschke and Bulla 2004). On the other hand, the number of baths does not play an essential role for methods such as quantum Monte Carlo where all the bath degrees of freedom are integrated out exactly and the calculations are performed for an effective (although very complicated) action. In this case, the number of degrees of freedom of the impurity site determines the computational effort (in addition to the values of Coulomb repulsion and temperature).

One fascinating aspect of the models in Fig. 3 is the appearance of *impurity quantum phase transitions* due to the competition of different physical mechanisms. A short review on this topic is given by Bulla and Vojta (2003). Impurity quantum phase transitions are a special class of so-called *boundary* quantum phase transitions (see Sec. 4 in Vojta (2003)) where only the degrees of freedom of a subsystem become critical (the impurity can be understood as a zero-dimensional boundary). Such impurity quantum phase transitions require the thermodynamic limit in the bath system, but are completely independent of possible *bulk* phase transitions in the bath.

Let us now come back to DMFT and the central issue of these lecture notes: the relation between quantum impurity physics and the physics of lattice models in DMFT. This issue shall be discussed in the context of the following three questions:

1. Is there a lattice counterpart for each possible type of quantum impurity model (which maps onto this quantum impurity model in DMFT)?
2. Which of the interesting features of quantum impurity systems can be found within DMFT? In particular: which quantum phase transitions and quantum critical points “survive” the DMFT self-consistency?
3. What are the new features of DMFT solutions for lattice models not present in the physics of quantum impurity models?

Question No. 1 cannot be answered in general. The situation is fairly clear for a class of models at the points $(0, M)$. As briefly mentioned above, multi-band Anderson models appear as effective impurity models in the DMFT for multi-band Hubbard models. Note that in this case the orbital structure of the lattice model shows up in both the impurity part and in the structure of the fermionic baths (Florens *et al.* 2002, Ōno *et al.* 2003, Pruschke and Bulla 2004, Rozenberg 1997).

The two-channel Kondo and Anderson lattices map on effective impurity models at the point $(0, 4)$ (Anders *et al.* 1997, Anders 1999). The non-Fermi liquid physics of the impurity models then shows up in the corresponding lattice models as well.

Models at $(N, 0)$ might appear as effective impurity models in a DMFT treatment of the Bose-Hubbard model, a bosonic version of the Hubbard model eq. (1) with the fermionic operators $c_{i\sigma}$ replaced by bosonic operators $b_{i\alpha}$ ($\alpha = 1, \dots, N$). This model has attracted renewed interest in the context of ultra-cold (bosonic) atoms in optical lattices (Jaksch *et al.* 1998). To our knowledge, the Bose-Hubbard model has not yet been treated within DMFT. The effective impurity models are presumably bosonic versions of the single-impurity Anderson model, occupying the points $(N, 0)$ in the diagram of Fig. 3. In this context, the recently observed Mott transition of ultra-cold atoms is of particular interest (Greiner *et al.* 2002); this Mott transition should then correspond to an impurity quantum phase transition in the bosonic single-impurity Anderson model; one of the questions arising here is whether a superfluid phase can at all be observed in such an effective impurity model.

It is not clear whether a DMFT for these bosonic Hubbard models would be as successful as the DMFT for fermionic models; but it is definitely worth to go in this direction and thereby possibly widen the range of applicability of the DMFT. Provided the basic questions concerning the DMFT for the bosonic Hubbard model can be solved, one might even think of an extension to mixtures of bosonic and fermionic atoms (see, for example, Goldwin *et al.* (2004) and references therein) which would place (within DMFT) the effective impurity models at the points (N, M) .

Another route to effective impurity models with both fermionic and bosonic baths is the *extended* DMFT (Si *et al.* 2001). This specific extension of DMFT is designed for the treatment of lattice models with both local and non-local interaction terms. A proper scaling of the non-local interaction term leads to an effective impurity model where the impurity couples to a fermionic bath (as usual) and, in addition, to a bosonic bath corresponding to spin fluctuations of the surrounding medium.

The extended DMFT has been applied to the Kondo lattice model (Grepel and Si 2003), the periodic Anderson model (Sun and Kotliar 2003) (both supplemented by a coupling between spins on neighbouring sites), the Hubbard model with long range Coulomb interactions (Chitra and Kotliar 2000), and the t - J -model (Haule *et al.* 2003). In all these cases, the effective impurity model is the Bose-Fermi Kondo model, with (depending on the details of the problem) three bosonic baths (including the SU(2)-symmetric case), two bosonic baths (including the XY-symmetric case) or one bosonic bath (the Ising case). For the Ising case, the Bose-Fermi Kondo model takes the form (Grepel and Si 2003, Zaránd and Demler 2002):

$$H = J\vec{S} \cdot \vec{s} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} \quad (6)$$

$$+ \frac{\sigma_z}{2} \sum_i \lambda_i (a_i + a_i^\dagger) + \sum_i \omega_i a_i^\dagger a_i . \quad (7)$$

This model is characterized by the competition between screening of the magnetic moment due to the coupling to the conduction band, and the coupling to the bosons which favour an unscreened spin. The resulting quantum phase transition and the connection to local criticality will be discussed further below.

To summarize the discussion of question No. 1, we observe that a full answer cannot be given at the moment and a lot of future work is needed, in particular in the context of bosonic models.

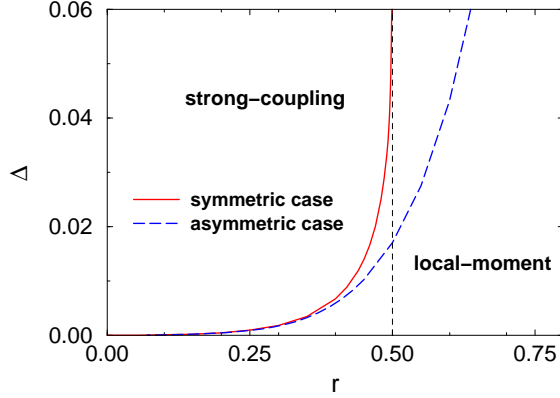


FIG. 4: $T = 0$ phase diagram for the soft-gap Anderson model in the p-h symmetric case (solid line, $U = 10^{-3}$, $\varepsilon_f = -0.5 \cdot 10^{-3}$, conduction band cutoff at -1 and 1) and the p-h asymmetric case (dashed line, $\varepsilon_f = -0.4 \cdot 10^{-3}$); Δ measures the hybridization strength, $\tilde{\Delta}(\omega) = \Delta|\omega|^r$ (Bulla *et al.* 2000, Gonzalez-Buxton and Ingersent 1998).

From this discussion it is obvious that question No. 2 is equally difficult to answer in general. Let us first consider the single-impurity Anderson model at $(0, 2)$ with a general bath spectral function, $\tilde{\Delta}(\omega) = \pi V^2 \sum_k \delta(\omega - \varepsilon_k)$, in particular the case of a soft-gap at the Fermi level: $\tilde{\Delta}(\omega) = \Delta|\omega|^r$, with an exponent $r > 0$ (Withoff 1990).

The soft-gap case $0 < r < \infty$ leads to a very rich behaviour, in particular to a continuous transition between a local-moment (LM) and a strong-coupling (SC) phase. Figure 4 shows a typical phase diagram for the soft-gap Anderson model. In the particle-hole (p-h) symmetric case (solid line) the critical coupling Δ_c diverges at $r = \frac{1}{2}$, and no screening occurs for $r > \frac{1}{2}$ (Bulla *et al.* (2000), Gonzalez-Buxton and Ingersent (1998)). No divergence occurs for p-h asymmetry (dashed line) (Gonzalez-Buxton and Ingersent 1998).

For further details on the quantum critical properties and the physics in the SC and LM phases see Bulla *et al.* (2000), Glossop and Logan (2003), Gonzalez-Buxton and Ingersent (1998), Vojta and Bulla (2002), Vojta (2003), Vojta and Fritz (2004).

Important for the present discussion is the appearance of a line of quantum critical points (solid and dashed lines in Fig. 4). Each quantum critical point on these lines has a structure of excitations which differs from both the SC and LM fixed points.

Obviously, the soft-gap models are only a sub-class of single-impurity models with a non-constant density of states. The question arises here whether such a soft-gap density of states appears in the effective impurity models within DMFT. So far, no example within

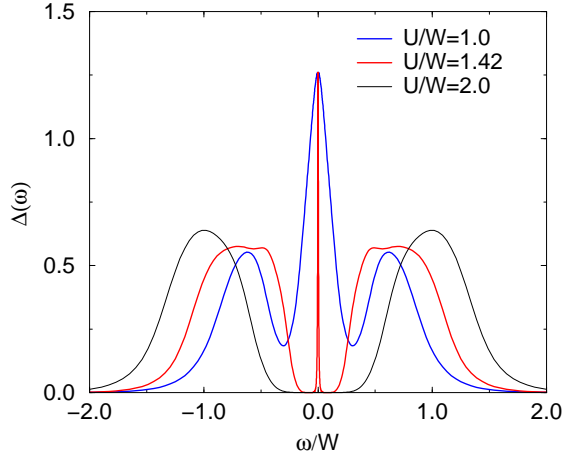


FIG. 5: Spectral functions for the Hubbard model on a Bethe lattice for various values of U (Bulla 1999). A narrow quasiparticle peak develops at the Fermi level which vanishes at the critical $U_c \approx 1.47W$ (with W the bandwidth of the non-interacting density of states).

DMFT has been found in which a soft-gap stabilizes itself under the DMFT iteration. Consequently, a lattice analogue of the soft-gap critical points has not yet been observed. (A soft-gap density of states might be generated in the DMFT solution of the Hubbard-Holstein model at the phase boundary between the metallic and the bipolaronic insulating state (Koller *et al.* 2004).)

Neglecting for a moment the appearance of a line of quantum critical points, the presence of both SC and LM phases in the impurity Anderson model does have a counterpart in DMFT, which is the well studied Mott transition in the Hubbard model.

Figure 5 shows the local spectral function for the particle-hole symmetric Hubbard model at $T = 0$ for different values of the local Coulomb repulsion U . These results are for the Bethe lattice (see Fig. 2 in Bulla (1999)); in this case, the local spectral function is proportional to the density of states of the free conduction band appearing in the effective single-impurity Anderson model.

The Mott transition at $T = 0$ is characterized by a vanishing of the quasiparticle peak at a value of $U \approx 1.47W$. On the metallic side of the transition, the $\Delta(\omega)$ approaches a constant for $\omega \rightarrow 0$, in other words, the low frequency behaviour corresponds to the $r = 0$ limit of the soft-gap Anderson model where no transition is observed and the system is always in the SC phase. On the insulating side of the transition, the $\Delta(\omega)$ shows a hard gap, corresponding to the $r \rightarrow \infty$ limit of the soft-gap Anderson model. For the p-h symmetric case, the system

is always in the LM phase for $r > 1/2$ so we conclude that the insulating side corresponds to the LM phase of the effective impurity model.

The Mott transition in DMFT shows the special feature that the quasiparticle peak vanishes continuously whereas the gap already has a finite value at the transition. Consequently, there is no quantum critical point separating the metallic from the insulating side. Instead, the transition point itself belongs to the insulating side and is not characterized by a critical spectrum of excitations.

The latter observation holds quite generally for all quantum phase transitions observed in lattice models within (standard) DMFT: no quantum critical behaviour has been reported so far. In any case, critical behaviour in DMFT cannot be due to non-local fluctuations; the only possibility is *locally* critical behaviour which has indeed been observed in the extended DMFT.

As discussed briefly above, a lattice model within extended DMFT (Si *et al.* 2001) is mapped onto one of the variants of the Bose-Fermi Kondo model. This model shows lines of quantum critical points when the bath spectral functions of the fermionic or bosonic baths follow a power-law at low energies (Kircan and Vojta 2004). The case of a sub-Ohmic bosonic bath is of special importance here. Let us concentrate on the Bose-Fermi Kondo model with Ising coupling to the bosonic bath and a constant density of states of the conduction electrons. This model can be mapped onto the spin-boson model with a bath spectral function which is the sum of an Ohmic (coming from the fermionic bath) and a sub-Ohmic part (Zhu *et al.* 2003). The quantum critical properties of this model are the same as for the pure sub-Ohmic spin-boson model which have been recently discussed in Bulla *et al.* (2003) and Vojta *et al.* (2004). Similar to the soft-gap Anderson model discussed above, the sub-Ohmic spin-boson model shows a line of quantum critical points for bath exponents $0 < s < 1$. The hyperscaling properties of this model, and the corresponding ω/T -scaling over the whole range of s values (Vojta *et al.* 2004) have direct consequences for the Kondo lattice model with Ising anisotropy. As discussed in Zhu *et al.* (2003), the criticality of the Bose-Fermi Kondo model is embedded in the criticality of the magnetic quantum phase transition of the Kondo lattice model.

Let us now turn to question No. 3. Some of the features of lattice models within DMFT *not* present in the physics of quantum impurity models are trivially connected to the existence of a lattice. This allows, for example, to define transport properties on the lattice

(Georges *et al.* 1996, Pruschke *et al.* 1995) and, in particular, the existence of long-range ordered phases which cannot have a direct counterpart in impurity models.

A typical example are antiferromagnetic phases in the Hubbard model which have been discussed in detail in Georges *et al.* (1996), Zitzler *et al.* (2002). Such a symmetry breaking does not exist in quantum impurity models. Furthermore, phase transitions in quantum impurity systems are restricted to *zero* temperature which is not the case in lattice models within DMFT. It turns out, however, that the mean-field nature of the DMFT determines the behaviour close to continuous (symmetry-breaking) transitions both at zero and finite temperature. As discussed in detail in Byczuk and Vollhardt (2002), only mean-field exponents for the vanishing of the order parameter or the divergence of the susceptibility can be observed, in agreement with numerical results (Jarrell 1992, Jarrell and Pruschke 1993).

Another example of a phase transition at finite temperature is the first order Mott transition in the Hubbard model (Bulla *et al.* 2001, Georges *et al.* 1996, 2004). The line of first order transitions terminates at a finite-temperature critical point, which has been discussed in detail in Georges *et al.* (2004). Physical properties such as the temperature dependence of the resistivity, $\rho(T)$, close to this critical end-point cannot have a direct counterpart in an effective impurity model. The reason is that for each temperature, the DMFT self-consistency results in a *different* quantum impurity model. The converged effective impurity models therefore change with temperature (and with all the model parameters).

CONCLUSIONS

The main focus of these lecture notes is on the relationship between quantum impurity models and lattice models within DMFT. Within the standard implementation of DMFT, a lattice model is mapped on an effective impurity model supplemented by a self-consistency condition. In this context, we discussed questions such as the observability of impurity quantum phase transitions in their lattice counterparts.

The DMFT for the simplest case where a lattice model maps on the single-impurity Anderson model is very well developed. Current topics of research are models involving additional degrees of freedom, such as multi-orbital Hubbard models in particular in the context of the LDA+DMFT approach (Held *et al.* 2003, Vollhardt *et al.* 2004), or bosonic degrees of freedom in the Holstein-Hubbard model (Koller *et al.* 2004). Another line of

active research are extensions of the “standard” DMFT: cluster extensions as reviewed in Maier *et al.* (2004), or the so-called extended DMFT (Si *et al.* 2001).

It should be mentioned here that other approaches exist within DMFT which do not depend on the mapping on an impurity model. One such approach is the Random Dispersion Approximation (Noack and Gebhard 1999) which has been applied to the Mott transition in the Hubbard model; in this approach the lattice model is simulated using a cluster with random hoppings between all lattice sites. Another more general attempt is based on the Luttinger-Ward functional (Potthoff *et al.* 2003). Here the solution of the lattice model is obtained via minimizing the grand potential in a space of trial self-energies.

Despite these possible alternative approaches, further progress in our understanding of quantum impurity systems is certainly very important for the future development of DMFT. This includes the need to further improve existing techniques and possibly to invent new techniques to investigate quantum impurity systems, in particular for systems with orbital and bosonic degrees of freedom.

Future work is necessary for a better understanding of local criticality (within extended DMFT), an example of quantum critical behaviour which, as discussed above, is found in both the lattice model and the corresponding impurity model. Some concerns about the ability of the extended DMFT to explain lattice quantum critical points have been raised recently (Kiránc and Vojta 2004); furthermore, non-analyticities in the theory might appear at low temperatures, as argued in Haule *et al.* (2003).

Future developments will certainly involve a fruitful interplay between investigations of quantum impurity models and lattice models within DMFT, and a variety of new applications of DMFT, for example to bosonic systems, are still lying ahead.

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